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Cyclotron excitations in pure bilayer graphene: Electron–hole asymmetry and Coulomb interaction

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ABSTRACT

Inter-Landau-level transitions in the bilayer graphene in high perpendicular magnetic field at the filling-factor $\nu = 0$ have been studied. The next-nearest-neighbor transitions, energy difference between dimer and non-dimer sites, and layer asymmetry are included. The influence of Coulomb interaction is taken into account. The magnetoplasmon excitations in bilayer graphene at small momenta are considered within the Hartree–Fock approximation. The asymmetry in cyclotron resonance of clean bilayer graphene is shown to depend on magnetic field. At lower magnetic fields the energy splitting in the spectrum is due to electron–hole one-particle asymmetry while at higher magnetic fields it is due to Coulomb interaction. For the fully symmetric case with half-filled zero-energy levels the energy splitting proportional to the energy of Coulomb interaction is found.

The bilayer graphene is the unique object which combines the parabolic dispersion law of quasiparticles near the zero energy point with the chirality exhibiting Berry phase 2π [1]. This picture is obtained with the tight-binding Hamiltonian for electrons taking into account only nearest-neighbor transitions; the one-electron spectrum is symmetric around zero energy. Taking into account next-nearest-neighbor transitions results in the asymmetry of electron spectrum around zero-energy point [2].

One-particle Landau levels in the bilayer graphene at high magnetic fields have been considered in the works [3,4] taking into account only nearest-neighbor transitions. For the bilayer with small asymmetry there are four weakly split two-fold degenerate levels near zero energy. The valley and orbital degeneracies are lifted, but the electron–hole symmetry is preserved. The near-zero-levels are strongly influenced by Coulomb electron–electron interaction.

The charge-density excitations at small momenta were considered theoretically within the Hartree–Fock approximation for monolayer graphene [5,6] and for bilayer [7]. In the works [8,9] electromagnetic response in graphene was calculated numerically in the RPA approximation for wide range of excitation momenta. In the works [10,11] intra-Landau level transitions were considered. The many-body corrections obtained within the renormalization method, including weak electron–hole asymmetry, and the attempts to explain sharp transition from square to linear dispersion regime were reported in Refs. [12–14]. In the works [5–7] Coulomb interaction was shown to conserve electron–hole symmetry for excitations.

In the present paper the inter-Landau-level transitions in the bilayer graphene in high perpendicular magnetic field at the filling-factor $\nu = 0$ are studied. The novelty of this work is that the electron–hole asymmetry and Coulomb interaction are included into consideration simultaneously. Special attention is given to the difference in the cyclotron transition energies for two valleys under different conditions. At lower magnetic fields the energy splitting is due to electron–hole one-particle asymmetry while at higher magnetic fields the energy splitting in the spectrum is due to Coulomb interaction.

The bilayer is modelled as two coupled hexagonal lattices with inequivalent sites (A1, B1) and (A2, B2) in the first and second graphene layers, arranged according to Bernal (A2–B1) stacking. In the tight-binding model the energy states of electrons in (A1–B2) dimer in the vicinity of zero-energy point are conveniently described by an effective two-component Hamiltonian [2–4]. The asymmetry between on-site energies in the two layers U arising from the influence of external gates or a doping effect, the next-nearest-neighbor transitions and the difference between on-site energies of dimer and non-dimer sites $\tilde{\Delta}$ are taken into account:

$$H = H_0 + H_1 + H_2; \quad H_0 = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} \tag{1}$$

$$H_1 = \frac{\xi U}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{1}{2m}\frac{\xi U}{\gamma_1}\begin{pmatrix} \pi^+\pi & 0 \\ 0 & -\pi\pi^+ \end{pmatrix} \tag{2}$$

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$$H_2 = \frac{1}{2m}\left(\frac{2\gamma_4}{\gamma_0} - \frac{\tilde{\Delta}}{\gamma_1}\right)\begin{pmatrix} \pi^+\pi & 0 \\ 0 & \pi\pi^+ \end{pmatrix} + \frac{\tilde{\Delta}}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (3)$$

where $\pi = \hbar k_x + i\hbar k_y$, $\pi^+ = \hbar k_x - i\hbar k_y$ are the complex momentum operators, $\mathbf{k}$ is the wave vector measured from the center of the valley, ξ is the valley index, $\xi = 1$ in the valley K, $\xi = -1$ in the valley K', γ_0 is the intra-layer A-B coupling parameter, γ_1 is the inter-layer A2-B1 coupling parameter, $m = \gamma_1/2v^2$ is the effective mass for bilayer graphene, $v = \frac{\sqrt{3}}{2\hbar}a\gamma_0$, a is the lattice constant.

The parameter γ_4 describes the next-nearest-neighbor transitions (A1–A2 and B1–B2 interlayer hopping), $\gamma_1 = 0.1\gamma_0$, $\gamma_4 = 0.05\gamma_0$.

H_0 is the basic term yielding a parabolic spectrum with the effective mass m. H_1 describes the layer asymmetry, leading to the opening of a gap $\sim U$ in the spectrum. H_2 is due to the next-nearest-neighbor transitions and the difference between on-site energies of dimer and non-dimer sites and is responsible for the electron–hole asymmetry in the spectrum around zero-energy point. The second term in H_2 results in the shift of the single-energy spectrum as a whole an will be omitted later. The two-component Hamiltonian is applicable if the considered electron energy $|\varepsilon|$ is within the energy range of $|\varepsilon| < \frac{1}{4}\gamma_1$. The weak asymmetry means that $U/\gamma_1 \ll 1$, $\Delta/\gamma_1 \ll 1$, $\gamma_4/\gamma_0 \ll 1$.

In the perpendicular magnetic field B the energy spectrum of Landau levels $E_{n\xi}$ ($n = 0,1,\pm N$, $N = 0,1,2,\ldots$) and corresponding two-component wave functions Ψ_{nk} are found from the Hamiltonian H using the Landau gauge $\mathbf{A} = (0,Bx)$, as in the work [4]. The magnetic length is $l_B = \sqrt{\hbar/eB}$, the cyclotron frequency is $\omega_c = eB/m$. The basis consisting of the wave functions describing the states in the ordinary two-dimensional electron gas $\phi_{Nk} = e^{iky}\phi_{Nk}(x)$ is used, where k is the parameter which labels degenerate states within one Landau level in Landau gauge:

$$E_0(\xi) = \frac{1}{2}\xi U, \quad E_1(\xi) = \frac{1}{2}\xi U - \xi\delta + \frac{2\gamma_4}{\gamma_0}\hbar\omega_c \quad (4)$$

$$E_{\pm N}(\xi) = \pm\hbar\omega_c\sqrt{N(N-1)} - \frac{1}{2}\xi\delta + \frac{\gamma_4}{\gamma_0}\hbar\omega_c(2N-1) \quad (5)$$

where $\delta = U\hbar\omega_c/\gamma_1$. $\Psi_{0k} = (\phi_{0k},0), \Psi_{1k} = (\phi_{1k},0)$, $\Psi_{nk} = a_n\phi_{Nk} + b_n\phi_{N-2,k}$. The coefficients a_n and b_n are the eigenvector components. Without any asymmetry in the zero approximation: $a_{\pm N} = 1/\sqrt{2}, b_{\pm N} = \pm 1/\sqrt{2}$.

Note that the spectrum of high-energy LLs is applicable for the fields and levels satisfying the condition $\hbar\omega_c\sqrt{N(N-1)} < \gamma_1/4$. For $\gamma_1 = 0.39$ eV this inequality yields $B < 50$ T for $N = 2$. For higher fields or higher levels the full four-band Hamiltonian has to be used to determine the exact LL spectrum. The Zeeman splitting is omitted. Although in graphite the electron g-factor is not small ($g = 2$), a very light effective mass $m \approx 0.054$ in the bilayer determines a small ratio between the Zeeman energy and LL splitting $\varepsilon_Z/\hbar\omega_c \sim 0.05$ [4]. Trigonal warping coming from $\gamma_3 = \gamma_{A1-B2} \ll \gamma_1$ is not included.

The Hamiltonian of the many-body system in the perpendicular magnetic field with the Coulomb interaction is

$$\hat{H} = \sum E_{n\xi}a^+_{\lambda\xi\sigma}a_{\lambda\xi\sigma} + H_{int} \quad (6)$$

where $a^+_{\lambda\xi\sigma}$ and $a_{\lambda\xi\sigma}$ are the one-particle creation and annihilation operators; $\lambda = (n,k)$, $n = 0, 1, \pm N$ indicates the Landau level; ξ and σ are valley and spin indexes:

$$H_{int} = \frac{1}{2}\sum V^{\lambda1;\lambda2}_{\lambda3,\lambda4}a^+_{\lambda4\xi\sigma}a^+_{\lambda3\xi'\sigma'}a_{\lambda2\xi'\sigma'}a_{\lambda1\xi\sigma} \quad (7)$$

The Coulomb interaction conserves spin and valley indexes. The matrix elements for Coulomb interaction are found using the two-component wave functions, as in Ref. [5] for monolayer graphene.

In this work only the charge-density-excitations are studied, valley and spin indexes (ξ,σ) are not changed. Corresponding operators for excitations (n,n') from the level n to the level n' with the momentum K are

$$Q^+_{n,n';\xi\sigma}(K) = \sum_k a^+_{\lambda'\xi\sigma}a_{\lambda\xi\sigma} \quad (8)$$

where $\lambda = (n,k)$, $\lambda' = (n',k+K)$. The magnetic field is high which means that $E_c \ll \hbar\omega_c$, E_c is the typical Coulomb energy: $E_c = e^2/\varepsilon l_B$. The momentum of excitation is small: $Kl_B \ll 1$. The problem is considered in the way analogous to that employed in Refs. [5,6] for monolayer graphene systems. The time-dependent Hartree–Fock approximation is used. The Hartree–Fock approach assumes that there is a small parameter $E_c/\Delta E_{nn'}(\xi) \ll 1$, where $\Delta E_{nn'}(\xi)$ is the transition energy without interaction $\Delta E_{nn'}(\xi) = E_{n'}(\xi) - E_n(\xi)$. For bilayer graphene $E_c = 10\sqrt{B}$, $\hbar\omega_c = 2.2B$ [3] and the ratio $\hbar\omega_c/E_c = 0.22B^{1/2}$ for $\epsilon = 5$. For the first high-energy transition $E_{12} \simeq \sqrt{2}\hbar\omega_c$, and therefore for $B = 40$ T the ratio $E_{12}/E_c \simeq 2$. We do not consider with this method the low-energy transitions between Landau levels 0 and 1 with energies close to zero.

The excitation energy $\tilde{E}_{n,n';\xi\sigma}$ consists of noninteracting and Coulomb parts:

$$\tilde{E}_{n,n';\xi\sigma} = \Delta E_{nn'}(\xi) + E^{ex}_{n,n'} + \Sigma_{n'\xi\sigma} - \Sigma_{n\xi\sigma} \quad (9)$$

Coulomb part is represented by the terms: "excitonic" $E^{ex}_{nn'}$ part due to direct interaction of the electron at the level n' and the hole at the level n and exchange self-energy $\Sigma_{n\xi\sigma}$ and $\Sigma_{n'\xi\sigma}$ corrections to the one-electron Landau level energies. The "depolarization" shift which is given in the random phase approximation (RPA) proportional to K is omitted. The restriction for $K \simeq 0$ enables to consider excitations with different (ξ,σ) independently. As for monolayer graphene, there is the problem of divergency of exchange self-energy Σ_n due to summation over all filled LLs.

The interlayer electron transitions from the top filled to the next free Landau levels with energies nearly ω_c are studied; the selection rules are $\Delta N = 1$. The case of filling-factor $\nu = 0$ is considered, it means the absence of free carriers or the equal amount of holes and electrons. Different possible ground states in magnetic field and different cyclotron transitions may correspond to this filling.

1. The asymmetric bilayer without e–h asymmetry

Let $U > 0$: In this case we have filling-factor $\nu = 4$ for the electrons in one valley and $\nu = 4$ for the holes in another valley. For the valley with $\xi = 1$ there is the top filled LL with $n = -2$ and the transition $(-2,1)$, and for the valley with $\xi = -1$ there are the top filled 0 and 1 LLs and the transition (1,2). Including spin there are two transitions of each type. The noninteracting part is the same for both types of transitions:

$$\Delta E_{-2,1}(1) = \Delta E_{1,2}(-1) = \omega_c\sqrt{2} + \tfrac{1}{2}|U - \delta| \quad (10)$$

Note that the electron–hole symmetry of one-particle Hamiltonian leads to the fact that $(-2,1)$ and (1,2) transitions are really the same and have the same energy. $(-2,1)$ in electron representation is (1,2) in hole representation. Taking into account spin degeneracy we have four transitions with equal energies. The small asymmetry is important only for filling of LLs and the wave functions may be used without asymmetry. For $\nu = 0$ integer filling the value of self-energy may depend on resolving the divergency problem, but it is not zero. There is no Kohn's theorem [15].

For the excitations in the different valleys energy splitting due to the layer asymmetry is absent.